**Indian Institute of Technology, Kharagpur**

Time: 45 minutes Full Marks: 10 No. of students: 40
Classtest 2 Autumn, 2010-2011 Department: Chemistry
Subject: CY40014 **Introduction to Computational Chemistry**

***Answer all questions***

Q.1 In chemical kinetics, it is often important to know the fraction of particles with a speed that exceeds a selected speed $v'$. According to collision theories of chemical kinetics, particles with a speed in excess of $v'$ are energetic enough to react and those with a speed less than $v'$ are not. Thus the fraction of particles capable of reacting in a gas phase reaction can be calculated using the Maxwell-Boltzmann distribution law as

$$f_{reactive} = 1.0 - \int_0^{v'} dv\, 4\pi v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)$$

Write a program to compute $f_{reactive}$ numerically using Simpson's one-third rule.

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Q.2. A student wrote the program shown on the right to fit a Lagrange polynomial $f(x) = \sum_{i=1}^{N} y_i \prod_{\substack{j=1 \\ j\neq i}}^{N} \frac{x - x_j}{x_i - x_j}$ of degree $N$ through an arbitrary number of data points $\{x_i, y_i\}$ $(i = 1, N)$. Write the corrected program calculate the value of *f(x)* at any value of *x* other than $\{x_i\}$'s given as input.

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```
implicit real*4 (a-h, o-z)
dimension y(100)
open(unit=14,file='data.in',status='old')
read(12,*)n
do i=1,n
  read(14,*)x(i),y(i)
end do
close(14)
open(unit=12,file='data2.in',status='old')
read(12,*)n
do j=1,n
  read(12,*)x(j)
end do
close(12)
read(*,*)x
sum=0.0

do i=1,n
do j=1,n
  if(i.ne.j)then
  prd=prd*((x-x(j))/(x(i)-x(j)))
  sum=sum+y(i)*prd
  end if
end do
end do

sum=fx
write(*,*)fx
stop
end
```